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Pseudogap in the normal state of cuprates.

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We show that underdoped cuprates are disordered materials with the diffusion coefficients of carriers as low as 10^{-5} $m^2.s^{-1}$. In these conditions Coulomb interaction between electrons must be taken into account. The main effect is to open a gap in the density of state (DOS) near the Fermi level (FL). We show that this model explains most of the observed features of the so-called "pseudogap" in the normal state and in particular its value, its anisotropy and its variation with doping.

1. INTODUCTION

Many experiments made in the normal state of high Tc superconductors (HTSC) have revealed a so-called pseudogap. This pseudogap was observed in transport, magnetic, specific heat measurements and in scanning tunneling and ARPES (angle resolved photoemission spectroscopy) measurements[1]. The description done in references [2-6] put it this way :

-"the pseudogap is mainly seen in the underdoped samples"

-"the pseudogap magnitude decreases with doping"

-"there is no normal-state pseudogap in overdoped samples"

-"the pseudogap is anisotropic in the CuO_2 planes, maximum in the $(0,\pm\pi)$ direction of the Brillouin Zone (B.Z.), minimum in the $(\pm\pi/2,\pm\pi/2)$ direction"

-"the pseudogap magnitude is temperature independent"

The pseudogap observed in the normal state seems to be a partial gap. It is related to a crossover temperature, named T*, below which its observation is possible. There is another crossover temperature named T°, which may be associated with a feature in the density of state (DOS). Many authors relate T* with magnetic phenomena (e.g. spin gap). But we have another explanation for the pseudogap related with T*. It is mainly observed in underdoped samples, which are disordered and in which the mean free path and thus the diffusion coefficient is very low. In these conditions, the diffusion length becomes of the order of magnitude or smaller than the electron wavelength $1/k_F$. The materials are thus disordered conductors and the Coulomb repulsion becomes important (for a review see Altshuler and Aronov[7]).

2. DESCRIPTION OF THE MODEL USED

Altshuler and Aronov[7] have developed a theory to study the effect of the electron-electron interaction on the properties of disordered conductors in the metallic conduction domain. The conditions for its application $k_F L_D << 1$ is also satisfied for underdoped cuprates (L_D is the diffusion length). The theory has also shown that the interaction effects are most clearly pronounced in low-dimensionality systems. We compute the one particle DOS taking into account the Coulomb interactions in the self-energy term. We show that particle repulsion produces a dip in the DOS at the Fermi energy. This dip is more pronounced in directions where the Fermi velocity is small. In the cuprates, where the Fermi surface is very anisotropic, we find that the pseudogap appears first in the directions of the saddle points (1,0) and equivalent of the CuO_2 planes. This is clearly seen in the ARPES experiments.

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We do the calculations in the following way. We take an anisotropic dispersion relation for the one electron energy ε_k in the CuO_2 planes (bidimensional):

$$\varepsilon_k = -2t(\cos X + \cos Y) + 4t' \cos X \cos Y + E_F - E_S \quad (1)$$

E_F is the FL energy, we take $E_F = 0$, and E_S is the saddle point energy, $X = k_x a$, $Y = k_y a$, $\mathbf{k}(k_x,k_y)$ is the wave vector.
The self-energy is computed using the following formula[7]:

$$\Sigma_m = \Sigma_m^{ex} + \Sigma_m^{H} \quad (2)$$

where Σ_m^{ex} is the exchange part and Σ^H_m the Hartree part of the self-energy.
The exchange energy is given by:

$$\Sigma_\varepsilon^{ex} = \frac{1}{2\pi\nu}\int_\varepsilon^\infty d\omega \int \frac{d^3q}{(2\pi)^3} U(\vec{q}) \frac{Dq^2}{\omega^2 + (Dq^2)^2} \quad (3)$$

with $\mathbf{q} = \mathbf{k'} - \mathbf{k}$, D the diffusion coefficient. $U(\mathbf{q})$ is the Fourier transform of the long range Coulomb interaction and the term in Dq^2 the Fourier transform of the electron-electron correlation function. For $U(\mathbf{q})$ we take a screened Coulomb potential (the screening is in tridimensional):

$$U(\mathbf{q}) = C / (q^2 + q_o^2) \quad (4)$$

where q_o^{-1} is the screening length. We then compute the DOS in the two directions (1,0) and (1,1) within a small angle $d\theta$, using a selfconsistent procedure.

3. VARIATION OF THE DIFFUSION COEFFICIENT D WITH DOPING (DISORDER) AND DIRECTION (ANISOTROPY)

In a simple Fermi liquid, the diffusion coefficient is given by $D = (1/3)v_F l$, v_F is the Fermi velocity and l is the mean free path. For a given sample, with doping and disordered fixed, l is constant and v_F varies with direction, it is much smaller near the saddle point A $(0,\pm\pi)$ than at point B $(\pm\pi/2,\pm\pi/2)$. Without Coulomb interaction, for a shift of the singularity energy (saddle point) from the Fermi energy, $E_F - E_S \approx 40$ meV for example, we find $v_F \approx 1.10^7$ cm.s^{-1} at point A, for $l \approx 10$ nm we estimate $D \approx 3.10^{-4}$ m^2.s^{-1}, and $v_F \approx 4.10^7$ cm.s^{-1} at point B. When the doping varies, l changes mainly due to the disorder and may be due to the impurities. In underdoped samples there are disorder in the oxygen vacancies and also crystalline defects. We assume that l is strongly reduced as the doping decreases until we reach a region where the crystalline order is restored in the insulating antiferromagnetic state. $E_F - E_S$ varies slightly and v_F at point A is reduced, v_F at point B remains almost unchanged, so the anisotropy remains.

We have done the calculations assuming that D is decreasing with decreasing doping.

4. RESULTS AND COMPARAISON WITH EXPERIMENTS

Our results are presented in figures [1-4]. We use the general following parameters:
- $q_o a$ (screening parameter) = 0.2
- t (transfer integral) = 0.25 eV
- ε_r (static dielectric constant) = 300
- cell's parameters (a,b,c) for a $La_{1-x}Sr_xCuO_4$ compound
- $E_F - E_S \approx 50$ à 40 meV (figs 1-4)

We use a finite lifetime of carriers to take into account the effect of disorder on the van Hove singularity ($\Gamma = 8$ meV).

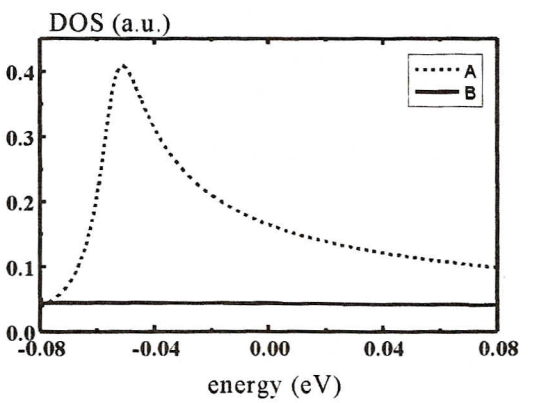

Figure 1. DOS without Coulomb interaction.
A : in the (1,0) direction, and equivalent directions
B : in the (1,1) direction
The strong increase of the DOS in the (1,0) direction is due to the effect of the saddle point.

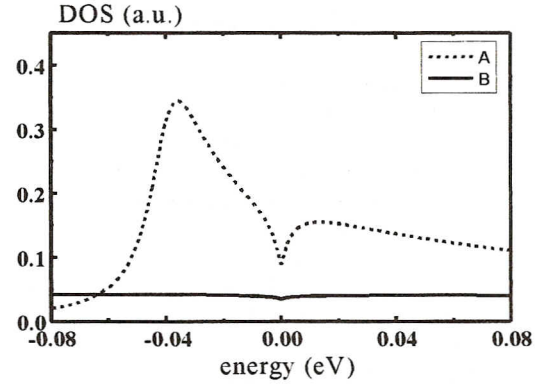

Figure 2. DOS with Coulomb interaction
A : in the (1,0) direction, and equivalent directions
and a diffusion coefficient D = 10^{-4} $m^2.s^{-1}$
B : in the (1,1) direction
and a diffusion coefficient D = 5.10^{-4} $m^2.s^{-1}$

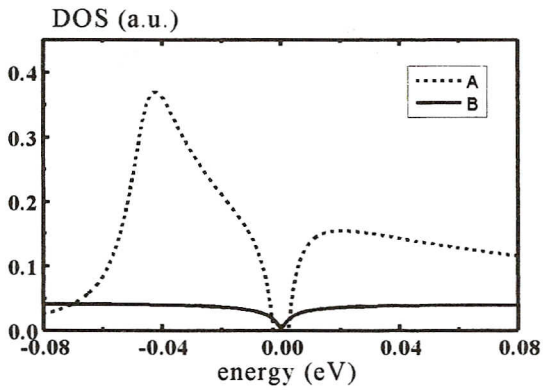

Figure 3. DOS with Coulomb interaction
A : in the (1,0) direction, and equivalent directions
and a diffusion coefficient D = 10^{-5} $m^2.s^{-1}$
B : in the (1,1) direction
and a diffusion coefficient D = 5.10^{-5} $m^2.s^{-1}$

We see clearly that the Coulomb repulsion opens a true gap in the (1,0) direction when D is small enough.

We can see from the figures [1-3] that our model explains why the pseudogap opens in the (1,0) direction and not in the (1,1) direction as seen in ARPES[2-5] .

In the review of Timusk and Statt[1], the authors give the values of estimated pseudogap from many experiments (fig. 50 ref. 7), the value for underdoped cuprates is around 40 meV. We obtain 20 meV for a screening parameter $q_o a = 0.2$, but for smaller value of $q_o a$ we can obtain a pseudogap of the order of 40 meV (figure 4). This shows that the screening is probably reduced in underdoped samples. We also see that the effect of a low screening is to put more states near the dip, forming maxima on the wings near it. This behavior can be related to the maxima observed in the scanning tunneling experiments[6].

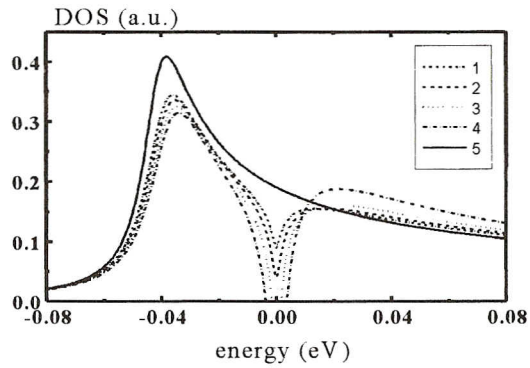

Figure 4.
Effect of the variation of the screening parameter.
with a diffusion coefficient D = 10^{-5} $m^2.s^{-1}$
1 : $q_o a = 0.2$
2 : $q_o a = 0.15$
3 : $q_o a = 0.10$
4 : $q_o a = 0.05$
5 : without interaction

5. CONCLUSION

Most of the authors relate the pseudogap to the superconductivity phenomena, because the behavior of both of them seams to be linked. But we want to notice that the pseudogap was observed in a non-superconducting region using scanning tunneling spectroscopy by T. Cren et al[8]. It means that the pseudogap can exist alone, and consequently it is not inevitably related to superconductivity, but it is an intrinsic property of the material. We have shown that the effect of the electron-electron interaction in disordered metallic conductors may explain it. Our next step will be the calculations through the Cooper pair channel to see the effect of Coulomb interactions on superconductivity.

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